学校编码：10384
学号：19820111152849

厦门大学

硕 士 学 位 论 文

一维Lennard-Jones气体的热传导行为

The Heat conduction of One-Dimensional Lennard_Jones Gas

马颖

指导教师：赵鸿

专业名称：理论物理

答辩日期：2014年5月

厦门大学学位论文原创性声明

本人呈交的学位论文是本人在导师指导下，独立完成的研究成果。本人在论文写作中参考其他个人或集体已经发表的研究成果，均在文中以适当方式明确标明，并符合法律规范和《厦门大学研究生学术活动规范（试行）》。

另外，该学位论文为（　　　　　　　　　　　　）课题（组）的研究成果，获得（　　　　　　　　　　　　）课题（组）经费或实验室的资助，在（　　　　　　）实验室完成。（请在以上括号内填写课题或课题组负责人或实验室名称，未有此项声明内容的，可以不作特别声明。）

声明人（签名）：

年　　月　　日

厦门大学学位论文著作权使用声明

本人同意厦门大学根据《中华人民共和国学位条例暂行实施办法》等规定保留和使用此学位论文，并向主管部门或其指定机构送交学位论文(包括纸质版和电子版)，允许学位论文进入厦门大学图书馆及其数据库被查阅、借阅。本人同意厦门大学将学位论文加入全国博士、硕士学位论文共建单位数据库进行检索，将学位论文的标题和摘要汇编出版，采用影印、缩印或者其它方式合理复制学位论文。

本学位论文属于：

(　　　)1.经厦门大学保密委员会审查核定的保密学位论文，于　年　月　日解密，解密后适用上述授权。

(　　　)2.不保密，适用上述授权。

(请在以上相应括号内打“√”或填上相应内容。保密学位论文应是已经厦门大学保密委员会审定过的学位论文，未经厦门大学保密委员会审定的学位论文均为公开学位论文。此声明栏不填写的，默认为公开学位论文，均适用上述授权。)

声明人(签名)：

年　　月　　日

摘 要

近几十年来，低维纳米材料和系统成为自然科学许多领域的研究前沿，其中，低维系统热传导行为研究是具有基础意义的研究课题。宏观三维材料的热传导由著名的傅里叶热传导定律描述，即热流正比于温度梯度： ，比例系数 为热传导率，是由材料性质决定的与材料尺寸无关的常数。这个定律在三维情况下早已被广泛验证，然而在低维系统中，虽然已经有一些初步的实验研究，但是实验精度还没有达到能给出明确结论的水平；而理论分析与数值模拟前期的研究都支持这样的预言：动量守恒的低维系统的热传导率随系统尺寸增长而增长，从而在热力学极限下发散。近年来，厦门大学复杂系统研究组提出了不同的观点，认为粒子间相互作用势的对称性对决定系统热输运行为具有关键作用，在相互作用势为非对称势的情况下，系统可能会表现出正常的热传导行为，热传导系数不依赖与系统尺寸。研究组已经进行了大量的研究，发现了许多确凿的例子，其中比较具有典型意义的是发现Lennard-Jones势一维晶格系统具有正常的热传导行为。

本文的主要目的是研究Lennard-Jones势一维气体模型的热传导行为。研究手段主要采用平衡态下计算热流涨落关联函数的弛豫行为，并利用Green-Kubo 公式计算热传导系数。为了验证所得到的结论，本文还将利用直接的非平衡数值模拟直接计算系统热传导系数对尺寸的依赖关系。本文的主要发现是Lennard-Jones势一维气体模型系统流关联衰减行为具有两个时间尺度，在非常短的尺度上首先经历快速的指数衰减过程，然后在大的时间尺度上经历指数衰减而趋于零关联。这不仅表明Lennard-Jones势一维气体具有正常的热传导行为，而且揭示了系统弛豫的准确过程。另外如果忽略了快速衰减过程，用Green-Kubo 公式计算热传导系数就不会准确。为了理解背后的微观动力学机制，本文还研究了气体粒子碰撞的动力学，发现和研究了这一模型系统中的混沌散射、非完全弹性散射、弹性散射以及随碰撞能量的过渡过程。

关键词：兰纳-琼斯势；热传导；Green-Kubo公式

Abstract

In recent decades, low-dimensional nano-materials and systems have been research frontiers in many fields of science, in which study of heat conduction in low-dimensional systems is of fundamental significance. Heat conduction in three-dimensional macroscopic materials can be described by the famous Fourier's law, i.e., the heat flow is proportional to the temperature gradient , where , heatconductivity, is intrinsic property of materials, irrespective of the size of material. Although the Fourier's law has been widely verified for three-dimensional cases, it is not experimentally conclusive for low-dimensional systems basically due to the precision of measurement in lab nowadays. On the other hand, results of theoretical analysis and molecular dynamical simulations of previous studies show that heatconductivity of momentum-conserving low-dimensional systems increases as the system size increases and diverges in the thermodynamic limit. However, the complex-system group of Xiamen University recently suggests that the asymmetry of the interaction potential plays a key role for the behavior of heat conduction. They show that normal conduction can be obtained for a system of asymmetric interaction potential based on extensive studies in several exemplified low-dimensional models, one of which is the one-dimensional lattice system with Lennard-Jones potential.

The main purpose of the presented thesis is to study the behavior of the heatconductivity of one-dimensional momentum-conserving gas model with Lennard-Jones potential. We compute the relaxation behavior of the heat flow's correlation function in the equilibrium state and then apply the Green-Kubo formula to calculate the heatconductivity. In order to verify the conclusion, we also use non-equilibrium molecular dynamical simulation to calculate the size dependence of thermal conductivity in a direct way. The main conclusion of the thesis is that the decay behavior of the flux correlation of the one-dimensional gas system with Lennard-Jones potential contains two time scales. The flux correlation exhibits a very rapid exponential-decay process in the first time scale and then be subjected to a slower exponential decay in the second time scale which is much longer. The results not only show that the one-dimensional gas model with Lennard-Jones potential has normal heat conduction but also reveal the exact relaxation process of the system. If the rapid-decay process was neglected, the calculation of thermal conductivity by the Green-Kubo formula would be incorrect. In order to understand the underlying microscopic mechanism, we also study the dynamics of the collision of particles and find chaotic scattering, non-completely elastic scattering, elastic scattering and the transition process of energy with the collision in the system.

Keywords: Lennard-Jones potential; heat conduction; Green-Kubo formula

参考资料

[1]Z. Rieder, J. L. Lebowitz, and E. Lieb, "Properties of a Harmonic Crystal in a Stationary Nonequilibrium State [J]," Journal of Mathematical Physics, vol. 8, pp. 1073-1078, 1967.
[2]B. J. Alder and T. E. Wainwright, "Decay of the Velocity Autocorrelation Function [J]," Physical Review A, vol. 1, pp. 18-21, 01/01/ 1970.
[3]S. G. Brush, The kind of motion we call heat [M]. Amsterdam: North-Holland, 1976.
[4]E. A. Jackson, "Nonlinearity and irreversibility in lattice dynamics [J]," Rocky Mountain J. Math, vol. 8, pp. 127-196, 1978.
[5]G. Casati, J. Ford, F. Vivaldi, and W. M. Visscher, "One-Dimensional Classical Many-Body System Having a Normal Thermal Conductivity [J]," Physical Review Letters, vol. 52, pp. 1861-1864, 05/21/ 1984.
[6]W. G. Hoover, "Canonical dynamics: equilibrium phase-space distributions [J]," Physical Review A, vol. 31, p. 1695, 1985.
[7]L. D. Landau and E. M. Lifshitz, Course of theoretical physics [M]: Pergamon Press, 1965.
[8]D. Forster, "Hydrodynamic fluctuations, broken symmetry, and correlation functions [M]," in Reading, Mass., WA Benjamin, Inc.(Frontiers in Physics. Volume 47), 1975. 343 p., 1975.
[9]L. P. Kadanoff and P. C. Martin, "Hydrodynamic equations and correlation functions [M]," Annals of Physics, vol. 24, pp. 419-469, 1963.
[10]M. T. R. Kubo, and N. Hashitsume, StatisticalPhysics II: Nonequilibrium Statistical Mechanics [M]. New York: Springer, 1991.
[11]N. Hashitsume, M. Toda, R. Kubo, and N. Sait ō , Statistical physics II: nonequilibrium statistical mechanics [M] vol. 30: Springer, 1992.
[12]H. Z. Cummins and R. W. Gammon, "Rayleigh and Brillouin scattering in liquids: the Landau—Placzek ratio [M]," The Journal of Chemical Physics, vol. 44, pp. 2785-2796, 2004.
[13]J. B. J. Fourier, Theorie Analytique de la Chaleur [M].Paris: Firmin Didot, 1822. English Translation in 1878 by Alexander Freeman. New York: Dover Publication, 2003.
[14]I. R. M. J. P. Hansen, Theory of simple liquids [M]. London: Academic Press, 2006.
[15]C. Kittel, Introduction to Solid State Physics [M]. New York: Wiey, 1996.
[16]R. G. Klages R, Sokolov I M, Anomalous Transport : Foundations and Applications [M]. Germany:Wiley-VCH Verlag GmbH &: Co. KgaA, Weinheim, 2008.
[17]M. C. R. Klages, Fractals and Transport in Nonequilibrium Statistical Mechanics [M]. Singapore: World Scientific, 2007.
[18]D. C. Rapaport, The art of molecular dynamics simulation [M]. Cambridge Cambridge University Press, 2004.
[19]S. D. Ross, "The interplanetary transport network [M]," 2006.
[20]陈式刚, 非平衡统计力学 [M]. 北京: 科学出版社, 2010.
[21]黄祖洽,丁鄂江, 输运理论 [M]. 北京: 科学出版社, 2008.
[22]"Focus issue: The Fermi-Pasta-Ulam problem-the first 50 years [J]," Chaos vol. 15, pp. 015101-015121, 2005.
[23]C. W. Chang, D. Okawa, H. Garcia, A. Majumdar, and A. Zettl, "Breakdown of Fourier ' s Law in Nanotube Thermal Conductors [J]," Physical Review Letters, vol. 101, p. 075903, 08/15/ 2008.
[24]L. Delfini, S. Lepri, R. Livi, and A. Politi, "Self-consistent mode-coupling approach to one-dimensional heat transport [J]," Physical Review E, vol. 73, p. 060201, 06/12/ 2006.
[25]L. Delfini, S. Lepri, R. Livi, and A. Politi, "Anomalous kinetics and transport from 1D self-consistent mode-coupling theory [J]," Journal of Statistical Mechanics: Theory and Experiment, vol. 2007, p. P02007, 2007.
[26]A. Dhar, "Heat transport in low-dimensional systems [J]," Advances in Physics, vol. 57, pp. 457-537, 2008/09/01 2008.

[27]O. Gendelman and A. Savin, "Normal heat conductivity of the one-dimensional lattice with periodic potential of nearest-neighbor interaction [J]," Physical Review Letters, vol. 84, p. 2381, 2000.
[28]C. Giardin à , R. Livi, A. Politi, and M. Vassalli, "Finite thermal conductivity in 1D lattices [J]," Physical Review Letters, vol. 84, p. 2144, 2000.
[29]P. Grassberger, W. Nadler, and L. Yang, "Heat conduction and entropy production in a one-dimensional hard-particle gas [J]," Physical Review Letters, vol. 89, p. 180601, 2002.
[30]B. Hu, B. Li, and H. Zhao, "Heat conduction in one-dimensional chains [J]," Physical Review E, vol. 57, pp. 2992-2995, 03/01/ 1998.
[31]B. Hu, B. Li, and H. Zhao, "Heat conduction in one-dimensional nonintegrable systems [J]," Physical Review E, vol. 61, pp. 3828-3831, 04/01/ 2000.
[32]F. issue, "The Fermi-Pasta-Ulam problem-the first 50 years [J]," Chaos 15, vol. 015101-015121, 2005.
[33]S. Lepri, R. Livi, and A. Politi, "Thermal conduction in classical low-dimensional lattices [J]," Physics Reports, vol. 377, pp. 1-80, 4// 2003.
[34]S. Lepri, R. Livi, and A. Politi, "Heat Conduction in Chains of Nonlinear Oscillators [J]," Physical Review Letters, vol. 78, pp. 1896-1899, 03/10/ 1997.
[35]J. Lukkarinen and H. Spohn, "Anomalous energy transport in the FPU - β chain [J]," Communications on Pure and Applied Mathematics, vol. 61, pp. 1753-1786, 2008.
[36]T. Mai, A. Dhar, and O. Narayan, "Equilibration and universal heat conduction in Fermi-Pasta-Ulam chains [J]," Physical Review Letters, vol. 98, pp. 1843011-184301_4, 2007.
[37]N. Mingo and D. A. Broido, "Length Dependence of Carbon Nanotube Thermal Conductivity and the "Problem of Long Waves" [J]," Nano Letters, vol. 5, pp. 1221-1225, 2005/07/01 2005.
[38]O. Narayan and S. Ramaswamy, "Anomalous Heat Conduction in One-Dimensional Momentum-Conserving Systems [J]," Physical Review Letters, vol. 89, p. 200601, 10/24/ 2002.
[39]A. Pereverzev, "Fermi-Pasta-Ulam β lattice: Peierls equation and anomalous heat conductivity [J]," Physical Review E, vol. 68, p. 056124, 2003.
[40]T. Prosen and D. K. Campbell, "Momentum conservation implies anomalous energy transport in 1D classical lattices [J]," Physical Review Letters, vol. 84, pp. 2857-2860, 2000.
[41]T. P. a. M. Robnik, "Energy transport and detailed verification of Fourier heat law in a chain of colliding harmonic oscillators [J]," Journal of Physics A: Mathematical and General, vol. 25, 1992.
[42]J.-S. Wang and B. Li, "Intriguing heat conduction of a chain with transverse motions [J]," Physical Review Letters, vol. 92, p. 074302, 2004.
[43]H. Zhao, "Identifying Diffusion Processes in One-Dimensional Lattices in Thermal Equilibrium [J]," Physical Review Letters, vol. 96, p. 140602, 04/14/ 2006.
[44]S. Chen, Y. Zhang, J. Wang, and H. Zhao, "Breakdown of the power-law decay prediction of the heat current correlation in one-dimensional momentum conserving lattices [J]," arXiv preprint arXiv:1204.5933, 2012.
[45]Y. Z. Shunda Chen, Jiao Wang, Hong Zhao, "Breakdown of the power-law decay prediction of the heat current correlation in one-dimensional momentum conserving lattices [J]," arXiv:1204.5933, 2012.
[46]Y. Zhong, Y. Zhang, J. Wang, and H. Zhao, "Normal heat conduction in one-dimensional momentum conserving lattices with asymmetric interactions [J]," Physical Review E, vol. 85, p. 060102, 06/20/ 2012.
[47]A. Dhar and K. Saito, "Anomalous transport and current fluctuations in a model of diffusing Levy walkers [J]," arXiv preprint arXiv:1308.5476, 2013.
[48]A. Savin and Y. A. Kosevich, "Thermal conductivity of the chain with an asymmetric pair interaction [J]," arXiv preprint arXiv:1307.4725, 2013.
[49]A. Savin, G. Tsironis, and A. Zolotaryuk, "Heat conduction in one-dimensional systems with hard-point interparticle interactions [J]," Physical review letters, vol. 88, p. 154301, 2002.
[50]N. D. M. N. W. Ashcroft Solid State Physics [M]. New York Saunders Colledge, 1988.
[51]R. E. Peierls, Quantum Theory of Solids [M]. London: Oxford University Press, 1955.

[52]J. L. L. F. Bonetto, L. Rey-Bellet, "Fourier's Law: a Challenge for Theorists [J]," Mathematical Physics, 2000.
[53]R. E. Peierls, Theoreticle Physics in the Twentieth Century [M] Edited by M. Fiera and V. F. Weisskopf. New York wiley, 1961.
[54]!!! INVALID CITATION !!!
[55]Y. Zhong, Y. Zhang, J. Wang, and H. Zhao, "Normal thermal conduction in lattice models with asymmetric harmonic interparticle interactions [J]," Chinese Physics B, vol. 22, p. 070505, 2013.
[56]H. van Beijeren, "Exact Results for Anomalous Transport in One-Dimensional Hamiltonian Systems [J]," Physical Review Letters, vol. 108, p. 180601, 04/30/ 2012.
[57]L. Wang and T. Wang, "Power-law divergent heat conductivity in one-dimensional momentum-conserving nonlinear lattices [J]," EPL (Europhysics Letters), vol. 93, p. 54002, 2011.
[58]S. Chen, Y. Zhang, J. Wang, and H. Zhao, "Diffusion of heat, energy, momentum, and mass in one-dimensional systems [J]," Physical Review E, vol. 87, p. 032153, 2013.
[59]J. Lebowitz, S. Olla, and G. Stoltz, "Nonequilibrium Statistical Mechanics: Mathematical Understanding and Numerical Simulation [J]," 2012.
[60]L. Wang, B. Hu, and B. Li, "Length dependence of heat conduction in one-dimensional lattices with asymmetric inter-particle interactions [J]," arXiv preprint arXiv:1308.6061, 2013.
[61]A. Dhar, K. Saito, and B. Derrida, "Exact solution of a L é vy walk model for anomalous heat transport [J]," Physical Review E, vol. 87, p. 010103, 2013.
[62]J. E. Lennard-Jones, "Cohesion [J]," Proceedings of the Physical Society, vol. 43, p. 461, 1931.
[63]J.-P. Hansen and L. Verlet, "Phase transitions of the Lennard-Jones system [J]," Physical Review, vol. 184, p. 151, 1969.
[64]D. J. Evans, "Thermal conductivity of the Lennard-Jones fluid [J]," Physical Review A, vol. 34, p. 1449, 1986.
[65]S. Lepri, P. Sandri, and A. Politi, "The one-dimensional Lennard-Jones system: collective fluctuations and breakdown of hydrodynamics [J]," The European Physical Journal B-Condensed Matter and Complex Systems, vol. 47, pp. 549-555, 2005.
[66]J. Yang, Y. Zhang, J. Wang, and H. Zhao, "Energy-transfer process in gas models of Lennard-Jones interactions [J]," Physical Review E, vol. 83, p. 052104, 2011.
[67]S. Sarman and D. J. Evans, "Heat flow and mass diffusion in binary lennard-jones mixtures [J]," Physical Review A, vol. 45, p. 2370, 1992.
[68]J. Ge, S. Kjelstrup, D. Bedeaux, J.-M. Simon, and B. Rousseau, "Transfer coefficients for evaporation of a system with a Lennard-Jones long-range spline potential [J]," Physical Review E, vol. 75, p. 061604, 2007.
[69]D. Levesque, L. Verlet, and J. K ü rkijarvi, "Computer" Experiments" on Classical Fluids. IV. Transport Properties and Time-Correlation Functions of the Lennard-Jones Liquid near Its Triple Point [J]," Physical Review A, vol. 7, p. 1690, 1973.
[70]W. G. Hoover, D. J. Evans, R. B. Hickman, A. J. Ladd, W. T. Ashurst, and B. Moran, "Lennard-Jones triple-point bulk and shear viscosities. Green-Kubo theory, Hamiltonian mechanics, and nonequilibrium molecular dynamics [J]," Physical Review A, vol. 22, pp. 1690-1697, 1980.
[71]A. McGaughey and M. Kaviany, "Thermal conductivity decomposition and analysis using molecular dynamics simulations. Part I. Lennard-Jones argon [J]," International Journal of Heat and Mass Transfer, vol. 47, pp. 1783-1798, 2004.
[72]T. Ikeshoji and B. Hafskjold, "Non-equilibrium molecular dynamics calculation of heat conduction in liquid and through liquid-gas interface [J]," Molecular Physics, vol. 81, pp. 251-261, 1994.
[73]L. Verlet, "Computer" experiments" on classical fluids. I. Thermodynamical properties of Lennard-Jones molecules [J]," Physical review, vol. 159, p. 98, 1967.
[74]陈顺达, "低维系统的扩散行为研究 [M]," 博士论文, 物理系, 厦门大学, 厦门, 2013.
[75]J.-P. Hansen and I. R. McDonald, Theory of simple liquids: Elsevier, 1990.
[76]朱建国,郑文琛,郑家贵,孙小松和王洪涛, 固体物理学 [M]. 北京: 科学出版社, 2005.
[77]C. Kittel, Introduction to Solid Physics [M]. New York: Wiley, 1996.

[78]周衍柏, 理论力学教程（第三版） [M]. 北京: 高等教育出版社, 2009.
[79]B. Duan, Z. Bai, and Y. Gu, "Chaotic scattering in collinear Ze-e-three-body Coulomb systems," Physical Review A, vol. 61, p. 062711, 2000.
[80]郝柏林, 从抛物线谈起———混沌动力学引论 [M] vol. 1. 北京: 北京大学出版社, 2013.
[81]S. N. Rasband, Dynamics: John Wiley & Sons, 1983.